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Actinide Cross Section Evaluations

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Abstract. The Livermore Computational Nuclear Physics group is charged with producing updated neutron incident cross section evaluations for all the actinides in the coming year, concentrating on neutron induced fission, neutron capture and (n,2n) cross sections. We attack this daunting task either by adopting other recent evaluations or by performing our own. Owing to the large number of nuclei involved, we seek to automate this process as much as possible. For this purpose, we have developed a series of computer codes: `x4i`, an interface to the EXFOR database, `fete`, a code that translates ENDF/B formatted evaluations into a computationally convenient form, and `da_fit`, a fitting code that takes all relevant EXFOR data for a reaction or set of reactions and performs a generalized least square fit to them, subject to various constraints and other prior information.

INTRODUCTION

Our goal is to produce the best possible evaluation for all neutron incident cross sections for all known actinides with uncertainty estimates. This is a daunting task that we approach from several directions. Fortunately this task is made easier due to the new ENDF/B-7 preliminary evaluations from LANL, the new JENDL-3.3 evaluations and the older, yet high quality, JEFF-3.0 and ENDF/B-6 evaluations. Still the evaluators in each of these cases did not always have access to the latest experimental data and our understanding of these nuclei often advances faster than our ability to perform evaluations. Thus, an automated approach to re-evaluating neutron induced reactions on these nuclei is needed. In these proceedings, we outline several new codes to facilitate this project and we outline our evolving approach to producing these evaluations. A summary of all evaluations and experimental data is available at [1].

We now outline our contribution. First, we describe our procedure for producing an evaluation. Second, we explain how we will perform our uncertainty estimates for modeled reactions. Next, we describe how we will perform fits to data where needed. Finally, we outline our future plans for this project.

EVALUATION PROCEDURE

Our first step in producing an evaluation is dividing a reaction into physically relevant energy ranges. For reactions with no threshold, these are the thermal region, resonance region, unresolved resonance region and the high energy region. For threshold reactions, we only need the high energy range. Because we need to automate this division, the energy ranges are fixed for all nuclei, even if the choices are not optimal for a given nucleus. Once we have performed this division, we examine how much data is available and how many evaluations have been performed for this nucleus and reaction and make a decision how to create an evaluation. We obtain all available data from the EXFOR database and translate them into a computationally convenient form using our `x4i` code [2]. We translate the existing evaluations into a similar form using Livermore's `fete` code [3].

If there is data in a particular energy range, then we must decide if there are enough data. We will do this by computing the mean spacing between data points and the variance in the data point spacing on this energy range:

$$\begin{aligned} \overline{\Delta E} &= (E_{\max} - E_{\min})/N_D \\ \mathrm{var}(\Delta E) &= \frac{1}{N_D(N_D-1)} \sum_{i=1}^{N_D} (E_{i+1} - E_i - \overline{\Delta E})^2 \end{aligned} \quad (1)$$

where N_D is the number of data points on the energy interval $(E_{\min}, E_{\max})$. If $\overline{\Delta E} < \overline{\Delta E}_{\mathrm{cut}}$ and $\mathrm{var}(\Delta E) < \mathrm{var}(\Delta E)_{\mathrm{cut}}$, then there is enough data and it evenly spaced enough to either choose a suitable evaluation or fit the data in the absence of a reasonable evaluation. To determine whether an evaluation is suitable, we compare the evaluation's χ^2/N_D to a predetermined parameter η_{cut} for this energy range:

$$\chi^2/N_D = \frac{1}{N} \sum_{i=1}^{N_D} \frac{\left(\sigma_i^{\mathrm{exp}} - \sigma^{\mathrm{eval}}(E_i)\right)^2}{(\delta\sigma_i^{\mathrm{exp}})^2}. \quad (2)$$

We then choose the evaluation with the lowest χ^2 from all of the suitable evaluations. The results from a test pass through the actinides is available in Ref. [1]. We comment that we did not compute covariance matrices for data, did not consider coupled (i.e. ratio) data and made no attempt to evaluate data itself. This implies that, for example, badly normalized data is not fixed. If no evaluation is suitable, then we will fit the data using our fitting code described below.

In many cases, there is no experimental data and there not much known about the nuclei in question. In these cases there is often only an evaluation either based on systematics (e.g. Livermore's older ENDL99 data) or an Hauser-Feshbach calculation (e.g. the newer ENDF/B-7 and some of the newer JENDL-3.3 evaluations). In this case we plan to just adopt the newest evaluation. This does not guarentee that we get the best evaluation, but there is no simple criteria on which we can base a computer algorithm. Because of this, we flag the evaluation for a follow up examination. Even with this simplifying choice, we still must produce uncertainty estimates. In the next section, we summarize the approach to uncertainty estimates from Ref. [4].

If there are no satisfactory evaluations and insufficient data, then we must consider performing our own Hauser-Feshbach calculations. We have not investigated this case thoroughly yet as it will require us to be able to drive an external Hauser-Feshbach code from within our framework. Furthermore, we must devise a consistency checking scheme, perhaps based on the amount of data available in either the ENSDF or RIPL databases. In any event, once we have performed our calculations, we must estimate the uncertainty on the computed cross sections. We discuss this in the next section.

UNCERTAINTY ESTIMATES FOR HAUSER-FESHBACH CALCULATIONS

For incident neutron energies below 20 MeV, reaction cross sections are mostly modeled with the Hauser-Feshbach model. This model takes several inputs: nuclear level schemes and level densities for all required nuclei, γ-ray strength functions, particle transmission coefficients and fission transmission coefficients (if using the Hill-Wheeler single or double humped barrier fission models). Estimating the uncertainty on modeled cross sections boils down to estimating the uncertainties on these components, then propagating the uncertainties.

In the Hauser-Feshbach model, a single-step reaction is given by

$$\sigma_i \sim \sigma_{\text{abs}} \frac{\Gamma_i}{\sum_j \Gamma_j}, \tag{3}$$

where σ_{abs} is the absorption cross section and Γ_i is the partial width for decaying into channel i. Hence $\text{BR}_i = \Gamma_i / \sum_j \Gamma_j$ is the branching fraction into channel i. Similarly, the $(n,2n)$ cross section (the only two-step reaction we consider) is given by

$$\sigma_{(\text{n,2n})} \sim \sigma_{\text{abs}} \frac{\Gamma_n^{A+1}}{\sum_j \Gamma_j^{A+1}} \frac{\Gamma_n^A}{\sum_j \Gamma_j^A} = \sigma_{\text{abs}} \text{BR}_n^{A+1} \text{BR}_n^A. \tag{4}$$

Here we have added the total nucleon number A as an index to remind ourselves which compound nucleus is relevant for each stage.

In either the one or two step case, the uncertainty on the absorption cross section is given by the optical model as we will discuss shortly. The partial widths are given by

$$\Gamma_i^A(E) \sim \int_0^{E-E_{\text{sep}}} d\varepsilon T_i(\varepsilon) \rho^A(E - E_{\text{sep}} - \varepsilon). \tag{5}$$

Here E_{sep} is the separation energy for this channel, T_i is the transmission coefficient for this channel and ρ is the level density for this compound nucleus. We estimate the relative uncertainty of the partial widths as

$$\frac{\delta \Gamma_i^A}{\Gamma_i^A} \sim \sqrt{\left(\frac{\delta T_i}{T_i}\right)^2 + \left(\frac{\delta \rho^A}{\rho^A}\right)^2}, \tag{6}$$

once we estimate the uncertainty in the level density.

We compute the particle transmission coefficients using an Optical Model Potential (OMP). The OMP is usually constrained by measurements of the total cross section and angular distributions from the elastic scattering. Since it is often straight-forward to measure the total cross section it is often possible to produce very high quality OMP's and hence predict the absorption and shape elastic cross sections. The total, absorption and shape elastic cross sections as well as the transmission coefficients are all related to the S-matrix:

$$\begin{aligned}
\sigma_{\text{tot}} &= \frac{2\pi}{k^2} \sum_\ell \left[(\ell+1)(1 - \text{Re} S_\ell^+) + \ell(1 - \text{Re} S_\ell^-) \right], \\
\sigma_{\text{abs}} &= \frac{\pi}{k^2} \sum_\ell \left[(\ell+1)(1 - |S_\ell^+|^2) + \ell(1 - |S_\ell^-|^2) \right], \\
\sigma_{\text{se}} &= \frac{\pi}{k^2} \sum_\ell \left[(\ell+1)|1 - S_\ell^+|^2 + \ell|1 - S_\ell^-|^2 \right], \\
T_\ell &= 1 - |S_\ell^\pm|^2.
\end{aligned} \tag{7}$$

Since the total cross section goes like one power of the S-matrix and the other parameters go like the S-matrix squared, we can expect that the relative uncertainty on these parameters is controlled by the uncertainty on the total cross section. Roughly speaking, we take:

$$\frac{\delta \sigma_{\text{abs}}}{\sigma_{\text{abs}}}, \frac{\delta \sigma_{\text{se}}}{\sigma_{\text{se}}}, \frac{\delta T_\ell}{T_\ell} \sim 2 \frac{\delta \sigma_{\text{tot}}}{\sigma_{\text{tot}}}. \tag{8}$$

We will estimate the uncertainty in the total cross-section by performing fits to the total cross section data and using systematics to extrapolate to other nuclei.

In order to estimate the uncertainty on the level density, we note that typically $\rho(E) \sim \rho_0 e^{E/T}$. Thus, the cumulative level distribution, $N(E)$, is given roughly by

$$N(E) = \int_0^{E_{\max}} dE \rho(E) \approx T\rho(E_{\max}). \tag{9}$$

Since we can count the cumulative level distribution directly by counting the levels in a given level scheme, we have an estimate of the level density. Furthermore, since $N(E)$'s uncertainty is $\delta N(E) = \sqrt{N(E)}$, we have a rough way to estimate the relative uncertainty on the level density:

$$\frac{\delta\rho(E)}{\rho(E)} \sim \frac{1}{\sqrt{N(E)}}. \tag{10}$$

Now let us combine these results to obtain the relative uncertainty on one-step and two-step compound nuclear cross sections. Under the assumption that the capture and fission channels have the same relative uncertainty as the particle exit channels, the uncertainty on the branching ratios is comparable to that of the partial widths: $\delta \mathrm{BR}_i/\mathrm{BR}_i \sim \delta\Gamma_i/\Gamma_i$. Strictly speaking the relative uncertainty on the partial widths is probably very different for the different channels, but lacking any better scheme we have made this crude assumption. With this approximation, the one-step and two-step compound cross sections have the following relative uncertainties:

$$\begin{aligned} \frac{\delta\sigma_{\text{one step}}}{\sigma_{\text{one step}}} &\sim \sqrt{2\left(\frac{2\delta\sigma_{\text{tot}}}{\sigma_{\text{tot}}}\right)^2 + \left(\frac{\delta\rho^{A+1}}{\rho^{A+1}}\right)^2}, \\ \frac{\delta\sigma_{(\text{n,2n})}}{\sigma_{(\text{n,2n})}} &\sim \sqrt{3\left(\frac{2\delta\sigma_{\text{tot}}}{\sigma_{\text{tot}}}\right)^2 + \left(\frac{\delta\rho^{A+1}}{\rho^{A+1}}\right)^2 + \left(\frac{\delta\rho^{A}}{\rho^{A}}\right)^2}. \end{aligned} \tag{11}$$

In this framework, multi-step fission should also be treated as a two or more step reaction.

In all cases, there are many sources of uncertainty in these cross sections so it is possible that we may arrive at a large model uncertainty. In these cases, we cap the relative uncertainty at 33% since this allows the modeled value to be consistent with zero at the 99% confidence level (corresponding to "3σ").

It is clear from Eqs. (3) and (4) that the cross section for a specific channel is related to all of the other channels through the sum over partial widths in the denominators. Given this, we must ask how to proceed in the case that we need to replace a badly modeled Γ_i with, say, a fit to data for that channel. This question is not academic: this problem occurs routinely for the fission cross sections. A little algebra shows that we can write a corrected cross section in terms of the corrected fission cross section and the uncorrected partial cross sections:

$$\sigma_{\text{x}}^{\text{fixed}} = \sigma_{\text{x}}^{\text{orig}} + \left(\sigma_{\text{f}}^{\text{orig}} - \sigma_{\text{f}}^{\text{fixed}}\right) \frac{\sigma_{\text{x}}^{\text{orig}}}{\sigma_{\text{ce}} + \sigma_\gamma + \sigma_{(\text{n,n'})} + \ldots}. \tag{12}$$

The sum in the denominator here runs over all open channels. The uncertainty resulting from the combination of this rescaling and previous modeling is given by:

$$\frac{\delta\sigma_{\text{x}}^{\text{fixed}}}{\sigma_{\text{x}}^{\text{fixed}}} \approx \sqrt{\left(\frac{\delta\sigma_{\text{x}}^{\text{orig}}}{\sigma_{\text{x}}^{\text{orig}}}\right)^2 + (\delta\sigma_{\text{f}}^{\text{fixed}})^2 \left(\frac{\sigma_{\text{x}}^{\text{orig}}/\sigma_{\text{x}}^{\text{fixed}}}{\sigma_{\text{ce}} + \sigma_\gamma + \ldots}\right)^2} \tag{13}$$

to leading order in the ratio $\sigma_{\text{x}}^{\text{orig}}/(\sigma_{\text{ce}} + \sigma_\gamma + \sigma_{(\text{n,n'})} + \ldots)$.

LEAST SQUARE FITS TO DATA

In those cases where we must fit data ourselves, we turn to our constrained generalized least-square inversion package `da_fit`. In addition to allowing for an off-diagonal covariance matrix in the data, `da_fit` can force the fitted cross sections to obey constraints such as:

$$\begin{aligned} \sigma_{\text{tot}}(E) &= \sigma_{\text{elas}} + \sigma_\gamma + \sigma_{\text{f}} + \sigma_{(\text{n,n'})} + \sigma_{(\text{n,2n})}, \\ \sigma_{(\text{n,2n})}(E_{\text{thresh}}) &= 0. \end{aligned} \tag{14}$$

This code is in active development and we hope to release it in the next fiscal year. In this code, we represent a cross section in a Basis Spline basis:

$$\sigma^{\text{fit}}(E) = \sum_{i=1}^{N_M} \sigma_i^{\text{fit}} B_i(E), \tag{15}$$

where σ_i^{fit} are the N_M coefficients of the spline that we fit and $B_i(E)$ is the spline basis. Basis Splines generalize box and linear splines to piece-wise polynomials of any order. In practice second order polynomials are sufficient because they allow for a smooth representation of fitted cross sections and allow us to impose constraints both on the value of the cross section and derivatives of the cross section.

To fit the data, we want to solve this equation in the least-square sense:

$$\sigma_i^{\text{data}} \equiv \sigma^{\text{data}}(E_i) = \sum_{j=1}^{N_M} \sigma_j^{\text{fit}} B_j(E_i), \tag{16}$$

where now $B_j(E_i)$ functions as the kernel of this matrix equation. We proceed as in Ref. [5] and find the vector of coefficients that minimize the χ^2:

$$\chi^2 = (B\cdot\sigma^{\text{fit}} - \sigma^{\text{data}})^T \cdot (\Delta^2\sigma^{\text{data}})^{-1} \cdot (B\cdot\sigma^{\text{data}} - \sigma^{\text{fit}}). \tag{17}$$

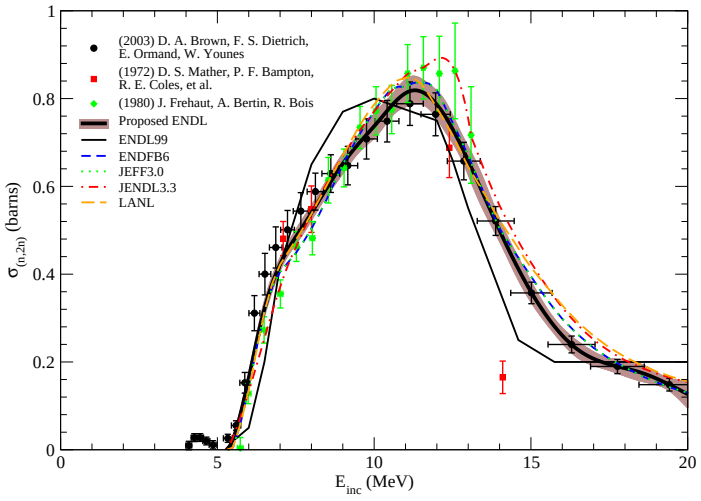

FIGURE 1. Fit to $^{235}\mathrm{U}(n,2n)$ data using 2^{nd} order Basis Spline, constraining the cross section to zero at threshold.

The coefficients that do this are:

$$\sigma^{\text{fit}} = \Delta^2\sigma^{\text{fit}} \cdot B^T \cdot (\Delta^2\sigma^{\text{data}})^{-1} \cdot \sigma^{\text{data}}. \qquad (18)$$

The covariance matrix of the fit coefficients is:

$$\Delta^2\sigma^{\text{fit}} = (B^T \cdot (\Delta^2\sigma^{\text{data}})^{-1} \cdot B)^{-1}. \qquad (19)$$

In order to stabilize the inversion, we can take advantage equality constraints. An equality constraint is a condition on the vector of fit coefficients that has the generic form $\mathscr{C} \cdot \sigma^{\text{fit}} = c$ such as in Eq. (14). Equality constraints are easily included by adding a penalty term to the χ^2: $\chi^2 + \lambda(\mathscr{C} \cdot \sigma^{\text{fit}} - c)^2$. Here λ is a trade-off parameter and we may vary it in order to emphasize stability in the inversion (by making λ huge) or to emphasize goodness-of-fit (by setting λ to zero). With this modification of the χ^2, the fit coefficients are

$$\sigma^{\text{fit}} = \Delta^2\sigma^{\text{fit}} \cdot \left(B^T \cdot (\Delta^2\sigma^{\text{data}})^{-1} \cdot \sigma^{\text{data}} + \lambda\mathscr{C}^T \cdot c\right), \qquad (20)$$

and the covariance matrix is

$$\Delta^2\sigma^{\text{fit}} = \left(B^T \cdot (\Delta^2\sigma^{\text{data}})^{-1} \cdot B + \lambda\mathscr{C}^T \cdot \mathscr{C}\right)^{-1}. \qquad (21)$$

An alternative approach is to use Lagrange multipliers to force the constraints to be obeyed. We have investiged this approach and found the results to be equivalent.

FUTURE PLANS

We have a lot of work to do to finish this project. Our main task is to implement various improvements to our fitter code, namely adding both fuzzy and inequality constraints and using the equations in the reaction fields of the EXFOR data to automatically assemble data covariance matrices. A secondary task is to either wrap an existing Hauser-Feshbach code or investigate the use of systematics when there is neither data nor an existing evaluation.

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